On a complexity of a spatial graph

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Abstract: In a research of proteins, molecules, or polymers, it is important to understand geometrically and topologicallyspatial graphs possibly with degree one vertices including knotted arcs. In this article, we introduce a concept of a complexity and related topological invariants for a spatial graph without degree one vertices , called the *γ-warping* and *warping degrees* as well as the *γ-unknotting* and *unknotting numbers* generalizing the usual unknotting number of a knot. These invariants define geometric invariants for a spatial graph with degree one vertices, meaningful even for a knotted arc.

1 A spatial graph without degree one vertices and its diagram

For general references of knots, links and spatial graphs, we refer to [3]. First, we consider a compact polygonal graph Γ which does not have any vertices of degrees 0 and 1 and, for simplicity, has at most one component with vertices of degrees $\geqq 3$. A *spatial graph* of Γ is a topological embedding image G of Γ into $\mathbf{R}^3$ such that there is an orientation-preserving homeomorphism $h : \mathbf{R}^3 \to \mathbf{R}^3$ sending G to a polygonal graph in $\mathbf{R}^3$. We consider a spatial graph G by ignoring the degree two vertices which are useless in our argument. When Γ is a loop, G is called a *knot*, and it is *trivial* if it is the boundary of a disk in $\mathbf{R}^3$. When Γ is the disjoint union of finitely many loops, G is called a *link*, and it is *trivial* if it is the boundary of mutually disjoint disks. A spatial graph G is *equivalent* to a spatial graph G' if there is an orientation-preserving homeomorphism $h : \mathbf{R}^3 \to \mathbf{R}^3$ such that $h(G) = G'$. Let $[G]$ be the class of spatial graphs G' which are equivalent to G. It is well-known that two spatial graphs G and G' are equivalent if and only if any diagram D_G of G is deformed into any diagram $D_{G'}$ of G' by a finite sequence of the generalized Reidemeister moves, where we call the moves necessary for links the *Reidemeister moves* (cf. [3]). Let $[D_G]$ be the class of diagrams obtained from a diagram D_G of G by the generalized Reidemeister moves, which is identified with the class $[G]$.

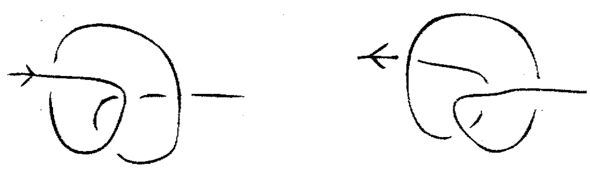

Figure 1: Monotone edge diagrams

2 A monotone diagram and complexity

Our spatial graph G is obtained from a maximal tree T (containing all the vertices of degrees $\geqq 3$ of G) by adding edges or loops α_i ($i = 1, 2, \cdots, m$). Clearly, $T = \emptyset$ if G is a link, and T is

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one vertex if G has just one vertex of degree $\geqq 3$. Let D be a diagram of G. The subdiagrams of D corresponding to T and α_i are called the *maximal tree diagram* DT and the *edge* or *loop diagram* $D\alpha_i$, respectively. Let $c_D(DT)$ be the number of crossing points of D belonging to DT. The diagram D is a *based diagram* (on T) and denoted by $(D;T)$ if $c_D(DT) = 0$. We can deform every diagram into a based diagram by a finite sequence of the generalized Reidemeister moves. Let $(D;T)$ be a based diagram of G, obtained from T by adding the edges or loops α_i $(i = 1, 2, \cdots, m)$. The edge diagram $D\alpha_i$ is *monotone* if there is an orientation on α_i such that a point going along the oriented diagram $D\alpha_i$ from the origin vertex meets first the upper crossing point at every crossing point (see Figure 1). The loop diagram $D\alpha_i$ is *monotone* if there is an orientation on α_i such that a point going along the oriented diagram $D\alpha_i$ from a non-crossing point always meets every upper crossing point first. The based diagram $(D;T)$ on T is *monotone* if $D\alpha_i$ is monotone for every i and contains the upper crossing point on every crossing point between $D\alpha_i$ and $D\alpha_j$ for any $j > i$ with respect to an oriented ordered sequence of $D\alpha_i$ $(i = 1, 2, \cdots, m)$. A similar notion of a monotone diagram was used by W. B. R. Lickorish and K. C. Millett in [5] for an oriented ordered link diagram. The *warping degree* $d(D;T)$ of a based diagram $(D;T)$ is the least number of crossing changes on the edge or loop diagrams $D\alpha_i (i = 1, 2, \cdots, m)$ needed to obtain a monotone diagram from D. For $T = \emptyset$, we denote $d(D;T)$ by $d(D)$. When the edges or loops α_i $(i = 1, 2, \cdots, m)$ are previpously oriented, we can also define the *oriented warping degree* $d^+(D;T)$ (or $d^+(D)$ for $T = \emptyset$) of D by considering only the crossing changes on the oriented edge or loop diagrams $D\alpha_i$ $(i = 1, 2, \cdots, m)$. For an oriented knot diagram D, A. Shimizu in [7] established the inequality $d^+(D) + d^+(-D) \leqq c(D) - 1$ with $c(D)$ the crossing number of D, where the equality holds if and only if D is an alternating diagram. The *complexity* of a based diagram (D,T) is the pair $cd(D;T) = (c(D;T), d(D;T))$ together with the dictionary order. This notion was introduced in [4] for an oriented ordered link diagram. A. Shimizu also observed that the dictionary order on $cd(D;T)$ is equivalent to the numerical order on $c(D;T)^2 + d(D;T)$ by using the inequality $d(D;T) \leqq c(D;T)$. The *complexity* $\gamma(G)$ of G is the minimum (in the dictionary order) of the complexities $cd(D;T)$ for all based diagrams $(D;T) \in [D_G]$. This topological invariant $\gamma(G)$ is also denoted by $(c_\gamma(G), \delta_\gamma(G))$ where $c_\gamma(G)$ and $\delta_\gamma(G))$ are called the *γ-crossing number* and the *γ-warping degree* of G, respectively. The minimal crossing number $c(G) = \min_{D \in [D_G]} c(D)$ of G has the inequality $c(G) \leqq c_\gamma(G)$. The following properties (1) and (2) on G gives a reason why we call $\gamma(G)$ the complexity of G:

(1) $c_\gamma(G) = 0$ if and only if $c(G) = 0$, i.e., G is equivalent to a graph in a plane. If $c_\gamma(G) > 0$, then there is a spatial graph G' with $c_\gamma(G') < c_\gamma(G)$ by a splice on G, so that $\gamma(G') < \gamma(G)$.

(2) $\delta_\gamma(G) = 0$ if and only if G is equivalent to G' with a monotone diagram $(D';T')$ with $c(D';T') = c_\gamma(G)$. If $\delta_\gamma(G) > 0$, then by a crossing change on G there is a spatial graph G' with $\gamma(G') < \gamma(G)$.

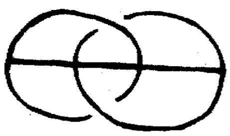

Figure 2: An unknotted plane graph with a Hopf constituent link

3 Warping degree and unknotting number

The *warping degree* $\delta(G)$ of G is the minimum of the warping degrees $d(D;T)$ for all based diagrams $(D;T) \in [D_G]$. Then $\delta(G)$ is a topological invariant and we have $\delta(G) \leqq \delta_\gamma(G)$. A spatial graph G is *unknotted* if $\delta(G)=0$, and γ-*unknotted* if $\delta_\gamma(G)=0$. A link L is unknotted in this sense if and only if L is a trivial link, and a spatial plane graph G is γ-unknotted if and only if G is equivalent to a graph in a plane. A *constituent link* of G is a link contained in G. We note that there is an unknotted plane graph with a non-trivial constituent link. For example, the spatial plane graph G in Figure 2 has $\delta(G)=0$, but has a Hopf constituent link and $\delta_\gamma(G)=1$. We also note the Conway-Gordon Theorem in [1]: Every spatial 6-complete graph K_6 contains a non-trivial constituent link, and every spatial 7-complete graph K_7 contains a non-trivial constituent knot. Nevertheless, we have the following properties on an unknotted graph: *For every graph Γ, there are only finitely many unknotted graphs G of Γ up to equivalences. Further, we have the following properties* (1) *and* (2) *on an unknotted graph G*: (1) *By a sequence of edge reductions illustrated in Figure 3, G is deformed into a maximal tree. In particular, every edge of G* is contained in a trivial constituent knot. (2) *G is equivalent to a trivial bouquet of circles after some edge contractions.* Let $u(D)$ be the minimal number of crossing changes of a diagram D needed to obtain a diagram of an unknotted graph. The *unknotting number* $\mu(G)$ of G is the minumum of the numbers $u(D)$ for all diagrams $D \in [D_G]$. Let $u_\gamma(D)$ be the minimal number of crossing changes of a diagram D needed to obtain a diagram of a γ-unknotted graph. The γ-*unknotting number* $\mu_\gamma(G)$ of G is the minumum of the numbers $u_\gamma(D)$ for all diagrams $D \in [D_G]$. The topological invariants $\mu(G)$, $\mu_\gamma(G)$, $\delta(G)$ *and* $\delta_\gamma(G)$ *are mutually distinct topological invariants satisfying the following square*:

$$\begin{array}{ccc} \mu_\gamma(G) & \leqq & \delta_\gamma(G) \\ \vee\!\| & & \vee\!\| \\ \mu(G) & \leqq & \delta(G) \end{array}$$

For example, the spatial graph G in Figure 2 has $\mu(G)=\delta(G)=0$ and $\mu_\gamma(G)=\delta_\gamma(G)=1$. On the other hand, we see that *Kinoshita's θ-curve* in Figure 4 has $\mu(G)=\mu_\gamma(G)=1<\delta(G)=\delta_\gamma(G)=2$ and $c(G)=4<c_\gamma(G)=7$. The proof of this assertion is omitted here, but our proof uses H. Moriuchi's classification of algebraic tangles in [6]. Also, we can show the following result by using a technique in [2]: *For every graph Γ and any integer $n \geqq 0$, there are infinitely many spatial graphs G of Γ such that $\mu(G)=\mu_\gamma(G)=\delta(G)=\delta_\gamma(G)=n$.*

4 A spatial graph with degree one vertices

Let Γ be a finite polygonal graph with degree 1 vertices, for simplicity, which has just one connected component with vertices of degrees $\geqq 3$. A *spatial graph* of Γ is a topological embedding image G of Γ into $\mathbf{R}^3$ such that $h(G)$ is a polygonal graph in $\mathbf{R}^3$ for an orientation-preserving

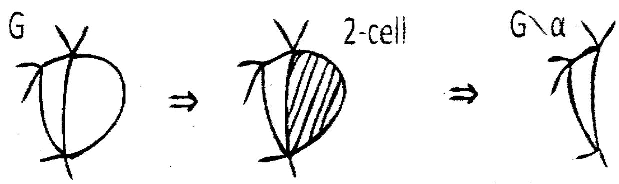

Figure 3: An edge reduction

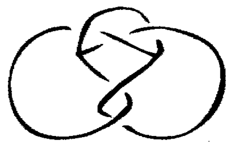

Figure 4: Kinoshita's θ-curve

homeomorphism $h : \mathbf{R}^3 \to \mathbf{R}^3$. Let V be the set of degree one vertices of G. For the line segment $[a,b]$ between $a, b \in \mathbf{R}^3$ and $x \in G$, let $S_v(x) = [v,x] \cup (\bigcup_{v,v' \in V} [v,v'])$ be a star with origin v. Assume that $G_v(x) = G \cup S_v(x)$ is a spatial graph without degree one vertices for every $v \in V$ and $x \in G$. Then the *warping degree* $\delta(G,x)$ and the *unknotting number* $\mu(G,x)$ of (G,x) are defined by $\delta(G,x) = \max_{v \in V} \delta(G_v(x))$ and $\mu(G,x) = \max_{v \in V} \mu(G_v(x))$, which are called the *warping degree* and the *unknotting number* of G and denoted by $\delta(G)$ and $\mu(G)$, respectively, when $x \in V$. An example is illustrated in Figure 5. In a similar way, the γ-*warping degrees* $\delta_\gamma(G,x)$, $\delta_\gamma(G)$ and the γ-*unknotting numbers* $\mu_\gamma(G,x)$, $\mu_\gamma(G)$ are defined. Different invariants taking the minimum or the average in place of the maximum are also defined.

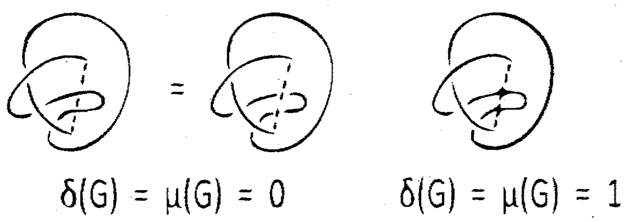

Figure 5: Knotted arcs

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